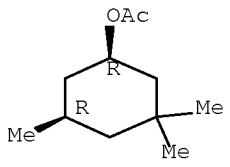
=> d ibib abs hitstr hitind l3 1-3

L3 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:1476435 HCAPLUS Full-text
TITLE: Essential oil constituents of the rhizomes of two types of Curcuma longa of Bangladesh
AUTHOR(S): Chowdhury, Jasim Uddin; Nandi, Nemai Chandra; Bhuiyan, M. Nazrul Islam; Mobarok, M. Hosnay
CORPORATE SOURCE: BCSIR Laboratories, Chittagong, 4220, Bangladesh
SOURCE: Bangladesh Journal of Scientific and Industrial Research (2008), 43(2), 259-266
CODEN: BJSIBL; ISSN: 0304-9809
PUBLISHER: Bangladesh Council of Scientific and Industrial Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Essential oil from the rhizomes of two types of Curcuma longa, yellow and red originated in Bangladesh was analyzed by GC-MS. 54 compds. have been identified from the yellow type of which the major compds. are ar-tumerone (27.78%), tumerone (17.16%), culone (13.82%), 2-carene (4.78%), zingiberene (4.37%) and β-sesquiphellandrene (5.57%). The red type contained 39 compds. with carvacrol (21.14%), citral (13.91%), methyleugenol (7.31%), geraniol (6.99%), menthol (5.11%) and caryophyllene oxide (4.14%) as major constituents.

IT INDEXING IN PROGRESS
IT 24691-16-5
RL: BSU (Biological study, unclassified); BIOL (Biological study) (cyclohexanol, 3,3,5-trimethyl-, acetate, cis- was present in essential oil of rhizome of red but not yellow type Curcuma longa of Bangladesh)
RN 24691-16-5 HCAPLUS
CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



CC 62-2 (Essential Oils and Cosmetics)
IT 24691-16-5
RL: BSU (Biological study, unclassified); BIOL (Biological study) (cyclohexanol, 3,3,5-trimethyl-, acetate, cis- was present in essential oil of rhizome of red but not yellow type Curcuma longa of Bangladesh)
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:96462 HCAPLUS Full-text
DOCUMENT NUMBER: 142:161998
TITLE: Cis-3,3,5-trimethylcyclohexyl esters for use as fragrances
INVENTOR(S): Kuhn, Walter; Surburg, Horst
PATENT ASSIGNEE(S): Symrise GmbH & Co. Kg, Germany
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005009492	A1	20050203	WO 2004-EP51292	200406 30
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10332908	A1	20050210	DE 2003-10332908	200307 19
EP 1648526	A1	20060426	EP 2004-741922	200406 30
EP 1648526	B1	20090909		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
AT 442166	T	20090915	AT 2004-741922	200406 30
US 20060211597	A1	20060921	US 2006-565241	200601 19

PRIORITY APPLN. INFO.:		DE 2003-10332908	A 200307 19
		WO 2004-EP51292	W 200406 30

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 142:161998
AB The invention relates to mixts. of cis-3,3,5-trimethylcyclohexyl esters with trans-3,3,5-trimethylcyclohexyl esters, the use of cis-3,3,5-trimethylcyclohexyl esters as fragrances and individual cis-3,3,5-

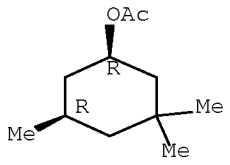
trimethylcyclohexyl esters and their use as fragrances. Thus 3,3,5-trimethylcyclohexyl acetate was synthesized from 3,3,5-trimethylcyclohexanol and acetic acid anhydride; the product contained 90% cis-3,3,5-trimethylcyclohexyl acetate. It was used in a fragrance composition as 65 weight part ingredient; other components were (weight parts): benzyl acetate 30; Ozonil (2-Tridecennitrile) 10% in diethylphthalate 5; dihydromyrcenol 150; decanal 1; 2-phenoxyethylisobutyrate 100; methylcedrylketon 35; hexyl cinnamic aldehyde 50; Lilial 30; linalyl acetate 100; Galaxolide 50% in diethylphthalate 10; cedryl acetate 30; Zibeth absolute synth. 1; lemon terpene 70; ethylvanillin 3; γ-undecalactone 1; citronitril 10; Projasmon P (2-heptylcycloheptanon) 1; Agrumex HC (2-tert.-butylcyclohexyl acetate) 30; hexenyl isobutyrate, cis/trans- 1; hexenylacetate cis/trans- 1; Limette oil, synth. 10; diethylphthalate 2.66.

IT 24691-16-5P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cis-3,3,5-trimethylcyclohexyl esters for use as fragrances)

RN 24691-16-5 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.

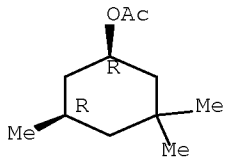


IPCI A61L0009-01 [ICM,7]; C07C0069-06 [ICS,7]; C07C0069-00 [ICS,7,C*]
IPCR C07C0069-00 [I,C*]; C07C0069-013 [I,A]
CC 62-2 (Essential Oils and Cosmetics)
IT 24691-16-5P 24691-18-7P 60234-70-0P 60234-71-1P
828912-37-4P 828912-38-5P 828912-39-6P 828912-40-9P
828912-41-0P 828912-42-1P 828912-44-3P 828912-46-5P
828912-48-7P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cis-3,3,5-trimethylcyclohexyl esters for use as fragrances)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1970:465956 HCAPLUS Full-text
DOCUMENT NUMBER: 73:65956
ORIGINAL REFERENCE NO.: 73:10799a,10802a
TITLE: Reductions with metal-ammonia combinations. II. Monothioacetals and monothioketals. Synthesis of alkoxymercaptans
AUTHOR(S): Eliel, Ernest L.; Doyle, Terrence W.
CORPORATE SOURCE: Dep. of Chem., Univ. of Notre Dame, Notre Dame, IN, USA
SOURCE: Journal of Organic Chemistry (1970), 35(8), 2716-22
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 73:65956
AB The reduction of oxathiolanes and oxathianes with metal-liquid NH3 combinations gives rise to β- and γ-alkoxymercaptans. Twenty-six cases were studied; yields are good for all oxathianes and most oxathiolanes (except those with very simple 2-alkyl groups) when the metal is Ca.
IT 24691-16-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24691-16-5 HCAPLUS
CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



CC 23 (Aliphatic Compounds)
IT 176-38-5P 4332-51-8P 5721-87-9P 10160-69-7P 10160-71-1P
10160-72-2P 10160-73-3P 10160-74-4P 10160-75-5P 10160-76-6P
10160-77-7P 10160-78-8P 16047-98-6P 16047-99-7P 17642-75-0P
17642-77-2P 17642-78-3P 17643-69-5P 17643-70-8P 24691-15-4P
24691-16-5P 24691-17-6P 24691-18-7P 24691-19-8P
24691-20-1P 24691-50-7P 24691-51-8P 24699-49-8P 24699-55-6P
24699-57-8P 24699-59-0P 24699-60-3P 24699-61-4P 24699-65-8P
24699-66-9P 24699-76-1P 24699-77-2P 24699-78-3P 24699-79-4P
24699-80-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS)

=> d ibib abs hitstr hitind l4 1-8

L4 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:756097 HCAPLUS Full-text
DOCUMENT NUMBER: 151:85996
TITLE: Use of 2,4'-dimethyl-propiophenone as a fragrance substance
INVENTOR(S): Kuhn, Walter; Lambrecht, Stefan; Panten, Johannes; Wiedmann, Willi
PATENT ASSIGNEE(S): Symrise G.m.b.H. & Co. K.-G., Germany
SOURCE: Eur. Pat. Appl., 22pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

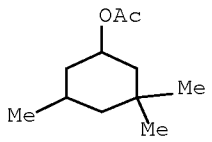
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

EP 2072083	A1	20090624	EP 2007-123731	200712 19
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS				
US 20090162308	A1	20090625	US 2008-337751	200812 18
PRIORITY APPLN. INFO.:			EP 2007-123731 A	200712 19

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 151:85996

AB The invention concerns the use of 2,4'-dimethylpropiophenone as a fragrance substance, preferably as a fragrance substance for imparting, modifying and/or reinforcing one, two, three or all the odor notes floral, rosy, rose oxide-like and herbal-like, preferably both of the odor notes rose oxide-like and herbal-like. Perfume, shampoo, antiperspirant, hair cosmetic and detergent compns. are exemplified that contain 2,4'-dimethyl-propiophenone as fragrance. Thus toluene and isobutyric acid chloride were reacted in the presence of aluminum chloride to obtain 2,4'-dimethyl-propiophenone with an isomer distribution of 94.4% para, 1.7 meta and 3.8 ortho isomer. A perfume composition contained (g): n-dodecanal 3; 2-methylundecanal 7; vertocitral 10; galbanum resin 3; styrolyl acetate 7; terpinylacetate 30; citral 10; Italian orange oil 20; Claritone 10; petit grain oil 20; lavandin oil 100; spikenard oil 100; rosemary oil 60; Spanish sage oil 30; dill oil 10; mugwort oil 10; Lyral 50; Hedione 50; methyloctine carbonate 1; Herbaflorate 25; herbylpropionate 20; Iso E Super 70; vetiver oil 10; veticol acetate 5; patchouli oil 30; Evernyl 5; Ambroxid crystalline 4; 2,4'-di-Me-propiophenone 70; dipropylene glycol 230.

IT 67859-96-5
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses) (in combination with; use of 2,4'-di-Me-propiophenone as a fragrance substance)
RN 67859-96-5 HCAPLUS
CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



IPCI A61Q0005-00 [I,A]; C11B0009-00 [I,A]; C07C0049-76 [I,A]; C07C0049-00 [I,C*]
IPCR A61Q0005-00 [I,C]; A61Q0005-00 [I,A]; C07C0049-00 [I,C]; C07C0049-76 [I,A]; C11B0009-00 [I,C]; C11B0009-00 [I,A]
CC 62-5 (Essential Oils and Cosmetics)
Section cross-reference(s): 5, 66
IT 60-12-8, 2-Phenylethyl alcohol 76-22-2, Camphor 78-69-3, Tetrahydrolinalool 78-70-6, Linalool 80-54-6, 2-Methyl-3-(4-tert-butylphenyl)propanal 87-44-5, Caryophyllene 88-41-5, 2-tert-Butylcyclohexyl acetate 90-17-5,

α-Trichloromethylbenzyl acetate 91-64-5, Coumarin 94-47-3, Phenylethylbenzoate 94-48-4, Geranylbenzoate 97-89-2, Citronellylisobutyrate 101-48-4, Phenylacetaldehyde dimethyl acetal 101-81-5, Diphenylmethane 101-84-8, Diphenyl oxide 101-86-0, α-Hexylcinnamic aldehyde 102-20-5, Phenylethylphenyl acetate 103-45-7 103-48-0 103-52-6 103-60-6, 2-Phenoxyethylisobutyrate 104-54-1, Cinnamic alcohol 104-62-1 105-85-1, Citronellyl formate 105-86-2, Geranyl formate 105-87-3, Geranyl acetate 105-90-8, Geranylpropionate 105-95-3, Ethylenebrassylate 106-02-5, Oxacyclohexadecan-2-one 106-21-8 106-22-9, Citronellol 106-24-1, Geraniol 106-25-2, Nerol 106-29-6, Geranylbutyrate 106-72-9, 2,6-Dimethyl-5-hepten-1-al 109-20-6, Geranylisovalerate 112-31-2, Decanal 112-43-6, 10-Undecenol 112-45-8, 10-Undecenal 115-95-7, Linalyl acetate 118-58-1, Benzylsalicylate 119-61-9, Benzophenone, biological studies 121-33-5, Vanillin 122-40-7 122-70-3, Phenylethylpropionate 122-78-1, Phenylacetaldehyde 127-41-3, α-Ionone 127-51-5, α-Isomethylionone 140-26-1, Phenylethylisovalerate 141-14-0, Citronellylpropionate 141-16-2, Citronellylbutyrate 150-84-5, Citronellyl acetate 470-82-6, 1,8-Cineol 498-16-8, Lavandulol 502-61-4, Farnesene 507-70-0, Borneol 562-74-3, 4-Terpinenol 1205-17-0, 2-Methyl-3-(3,4-methylenedioxyphenyl)propanal 1817-90-9 1860-40-8 2345-26-8, Geranylisobutyrate 2500-83-6 2565-82-4, Geranylmethyl ether 2630-39-9, Methyldihydrojasmonate 3391-86-4, 1-Octen-3-ol 3558-60-9 3681-71-8, cis-3-Hexenyl acetate 3681-82-1, trans-3-Hexenylacetate 3796-70-1, Geranylacetone 4602-84-0, Farnesol 4707-47-5 4941-78-0, Oxacyclohexadec-13-en-2-one 5413-60-5, 4,7-Methano-3a,4,5,6,7,7a-hexahydro-6-indenyl acetate 6259-76-3, Hexylsalicylate 6315-04-4 7212-44-4, Nerolidol 7492-67-3, Citronellyloxyacetaldehyde 7779-30-8 7785-33-3, Geranyl tiglate 8000-41-7, Terpineol 8007-35-0, Terpinyl acetate 10339-55-6, Ethyllinalool 10482-77-6, Citronellylbenzoate 10522-41-5 13019-22-2, 9-Decenol 16409-43-1, Roseoxide 20777-39-3, Lavandulyl acetate 21145-77-7 21944-94-5 23726-91-2, β-Damascone 23726-93-4, β-Damascenone 24717-85-9, Citronellyl tiglate 25225-10-9 25634-93-9, 2-Methyl-5-phenylpentanol 28069-72-9, trans-2,cis-6-Nonadienol 28219-61-6, 2-Ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol 28940-11-6 31906-04-4, 4-(4-Hydroxy-4-methylpentyl)-3-cyclohexenecarboxaldehyde 32210-23-4, 4-tert-Butylcyclohexyl acetate 32539-78-9, Oxacyclohexadec-12-en-2-one 33673-71-1 35087-49-1, γ-Damascone 36613-11-3 41199-19-3 43052-87-5, α-Damascone 50816-18-7, 9-Decenyl acetate 53219-21-9, Dihydromyrcenol 54464-57-2 54546-26-8, 2-Butyl-4,4,6-trimethyl-1,3-dioxane 55066-48-3, 3-Methyl-5-phenylpentanol 55719-85-2, 2-Phenylethyl tiglate 56011-02-0, Phenylethylisoamylether 57378-68-4, δ-Damascone 63500-71-0 64988-06-3 67634-15-5, 3-(4-Ethylphenyl)-2,2-dimethylpropanal 67662-96-8, Phenethyl pivalate 67859-96-5 68039-49-6, 2,4-Dimethyl-3-cyclohexenecarboxaldehyde 68527-77-5 68922-10-1, Citronellylisovalerate 70024-54-3 74338-72-0, 2,4,4,7-Tetramethyloct-6-en-3-one 101151-17-1 125109-85-5, 3-(3-Isopropylphenyl)butanal 135546-43-9 145206-68-4
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(in combination with; use of 2,4'-di-Me-propiophenone as a

fragrance substance)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:46762 HCAPLUS Full-text
DOCUMENT NUMBER: 150:128383
TITLE: Use of menthyl methyl ether and additional ethers to provide a feeling of cleanliness and purity especially with deodorants
INVENTOR(S): Kurzenne, Pierre; Collas, Violaine; Favre-Bulle, Beatrice; Machinek, Arnold; Surburg, Horst
PATENT ASSIGNEE(S): Symrise G.m.b.H. & Co. K.-G., Germany
SOURCE: Eur. Pat. Appl., 32pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 2014273	A1	20090114	EP 2007-110259	20070614

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS

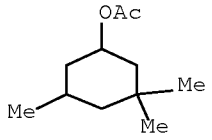
PRIORITY APPLN. INFO.: EP 2007-110259 20070614

OTHER SOURCE(S): MARPAT 150:128383

AB The invention concerns the use of a menthyl Me ether or a mixture of two or more menthyl ethers in cosmetic formulations in order to improve the feeling of cleanliness and purity. Thus a composition contained (weight parts): L-menthylmethyl ether 200; Florazon 10; Frescomenthe 30; peppermint oil 10; L-menthol 200; L-carvone 10; Calone 1951 1; Hedione 50; Anethol 5; Iso E Super 100; Ambrinol S 3; isomenthyl acetate 50; dipropylene glycol 330.

IT 67859-96-5
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(in combination with; use of menthyl Me ether and addnl. ethers to provide a feeling of cleanliness and purity especially with deodorants)

RN 67859-96-5 HCAPLUS
CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



IPCI A61K0008-04 [I,A]; A61K0008-33 [I,A]; A61K0008-30 [I,C*]; A61Q0013-00 [I,A]; A61Q0015-00 [I,A]

CC 62-4 (Essential Oils and Cosmetics)
IT 78-69-3, Tetrahydrolinalool 80-54-6,
2-Methyl-3-(4-tert-butylphenyl)propanal 88-41-5,
2-tert-Butylcyclohexyl acetate 91-64-5, Coumarin 101-86-0,
α-Hexylcinnamic aldehyde 103-60-6, 2-Phenoxyethylisobutyrate
104-54-1, Cinnamic alcohol 105-95-3, Ethylenebrassylate
106-02-5, Oxacyclohexadecan-2-one 106-22-9, Citronellol 106-72-9
115-95-7, Linalyl acetate 118-58-1, Benzylsalicylate 121-33-5,
Vanillin 122-40-7 127-41-3, α-Ionone 127-51-5,
α-Isomethylionone 1205-17-0 1222-05-5, Galaxolide
2500-83-6 2630-39-9, Methyldihydrojasmonate 3681-71-8,
cis-3-Hexenyl acetate 3681-82-1, trans-3-Hexenyl acetate
4941-78-0, Oxacyclohexadec-13-en-2-one 5413-60-5, Herbaflorat
6259-76-3, Hexylsalicylate 7779-30-8 8007-35-0, Terpinyl acetate
10339-55-6, Ethyllinalool 10522-41-5 14765-30-1,
2-sec-Butylcyclohexanone 21145-77-7 21944-94-5 22457-23-4
28069-72-9, trans-2,cis-6-Nonadienol 28219-61-6,
2-Ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol
28940-11-6 32210-23-4, 4-tert-Butylcyclohexyl acetate
32539-78-9, Oxacyclohexadec-12-en-2-one 41199-19-3 53219-21-9,
Dihydromyrcenol 54464-57-2 54464-57-2, Iso E Super 63500-71-0
67634-15-5, 3-(4-Ethylphenyl)-2,2-dimethylpropanal 67715-80-4,
2-Methyl-4-propyl-1,3-oxathiane 67859-96-5 68039-49-6,
2,4-Dimethyl-3-cyclohexenecarboxaldehyde 74338-72-0 101151-17-1
125109-85-5 130066-44-3, Lyral
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(in combination with; use of menthyl Me ether and addnl. ethers
to provide a feeling of cleanliness and purity especially with
deodorants)
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN
THE RE FORMAT

L4 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:1243858 HCAPLUS Full-text
DOCUMENT NUMBER: 149:424509
TITLE: Cooling compositions including menthyl esters
INVENTOR(S): Kiefer, Jesse; Harvey, Joan E.
PATENT ASSIGNEE(S): Cadbury Adams USA LLC, USA
SOURCE: PCT Int. Appl., 53pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008124667	A1	20081016	WO 2008-US59530	20080407

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY,
BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE,
EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN,
IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT,
LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK,
SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,

VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

US 20070221236	A1	20070927	US 2007-732942	200704 05
EP 2129234	A1	20091209	EP 2008-745205	200804 07

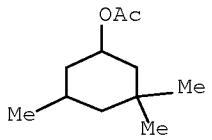
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR

PRIORITY APPLN. INFO.:	US 2007-732942	A 200704 05
	US 2005-723698P	P 200510 05
	US 2006-543473	A2 200610 05
	WO 2008-US59530	W 200804 07

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB Cooling compns. deliver a prolonged physiol. cooling sensation to the skin or a mucous membrane. The cooling compns. may be present alone or in product such as a chewing gum or a confection. In some embodiments, the cooling compns. include menthyl glutarate and at least one addnl. cooling agent, which may be WS-3 or WS-23, and optionally menthol. The cooling compns. may be in a liquid form at room temperature Thus, a cooling composition includes menthyl glutarate 5-60, WS3 or WS23 5-50, and menthol 15-85 % weight/weight

IT 67859-96-5
RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses) (cooling compns. including menthyl esters and chewing gums comprising these)
RN 67859-96-5 HCAPLUS
CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



IPCI A23G0004-00 [I,A]; A23G0004-18 [I,A]; A61K0009-68 [I,A]
IPCR A23G0004-00 [I,C]; A23G0004-00 [I,A]; A23G0004-18 [I,C]; A23G0004-18 [I,A]; A61K0009-68 [I,C]; A61K0009-68 [I,A]
CC 17-6 (Food and Feed Chemistry)
IT 89-78-1 89-79-2 1490-04-6D, esters 2623-23-6 16409-45-3

17162-29-7 34212-59-4 39711-79-0 42822-86-6 51115-67-4
67859-96-5 77304-30-4 77341-67-4 185915-25-7
220621-22-7 930287-43-7
RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(cooling compns. including menthyl esters and chewing gums
comprising these)
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2007:1093006 HCAPLUS Full-text
DOCUMENT NUMBER: 147:384825
TITLE: Cooling compositions including menthyl esters
INVENTOR(S): Kiefer, Jesse; Harvey, Joan E.
PATENT ASSIGNEE(S): Cadbury Adams USA LLC., USA
SOURCE: U.S. Pat. Appl. Publ., 20pp., Cont.-in-part of U.S. Ser. No. 543,473.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070221236	A1	20070927	US 2007-732942	20070405
AU 2006302337	A1	20070419	AU 2006-302337	20061005
CA 2623545	A1	20070419	CA 2006-2623545	20061005
WO 2007044526	A2	20070419	WO 2006-US39158	20061005
WO 2007044526	A3	20070628		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
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EP 1962779	A2	20080903	EP 2006-825560	20061005
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JP 2009519003 T 20090514 JP 2008-534717
200610
05
IN 2008KN01197 A 20080905 IN 2008-KN1197
200803
24
MX 2008004307 A 20080409 MX 2008-4307
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CN 101282707 A 20081008 CN 2006-80037226
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WO 2008124667 A1 20081016 WO 2008-US59530
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VN, ZA, ZM, ZW
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NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ,
TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
EP 2129234 A1 20091209 EP 2008-745205
200804
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R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR,
HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO,
SE, SI, SK, TR
PRIORITY APPLN. INFO.: US 2005-723698P P
200510
05
US 2006-543473 A2
200610
05
WO 2006-US39158 W
200610
05
US 2007-732942 A
200704
05
WO 2008-US59530 W
200804
07

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

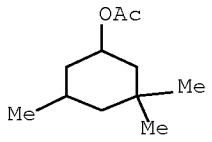
AB Cooling compns. deliver a prolonged physiol. cooling sensation to the skin or a mucous membrane. The cooling compns. may be present alone or in product such as a chewing gum or a confection. In some embodiments, the cooling compns. include menthyl glutarate and at least one addnl. cooling agent, which may be WS-3 or WS-23, and optionally menthol. The cooling compns. may be in a

liquid form at room temperature Thus, a cooling composition includes menthyl glutarate 5-60, WS3 or WS23 5-50, and menthol 15-85 % weight/weight

IT 67859-96-5, Homomenthyl acetate
RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(cooling compns. including menthyl esters and chewing gums comprising these)

RN 67859-96-5 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



INCL 131352000
IPCI A24B0015-00 [I,A]
IPCR A24B0015-00 [I,C]; A24B0015-00 [I,A]
NCL 131/352.000
CC 17-6 (Food and Feed Chemistry)

IT 89-78-1, Menthol 89-79-2, L-Isopulegol 1490-04-6D, Menthol, esters 2623-23-6, L-Menthyl acetate 16409-45-3, Menthyl acetate 17162-29-7, Menthyl lactate 34212-59-4 39711-79-0, WS-3 42822-86-6, p-Menthane-3,8-diol 51115-67-4, WS-23 67859-96-5, Homomenthyl acetate 77304-30-4 77341-67-4 185915-25-7, L-Menthyl lactate 220621-22-7 930287-43-7
RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(cooling compns. including menthyl esters and chewing gums comprising these)

L4 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2001:452890 HCAPLUS Full-text
DOCUMENT NUMBER: 135:66066
TITLE: Ester odor neutralizers
INVENTOR(S): Rohde, Ute; Hillers, Stephan; Surburg, Horst; Sonnenberg, Steffen; Mcdermott, Keith; Smith, Leslie; Sparkuhle, Karl
PATENT ASSIGNEE(S): Haarmann & Reimer G.m.b.H., Germany; Haarmann und Reimer G.m.b.H.
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001043784	A2	20010621	WO 2000-EP12374	200012 08
WO 2001043784	A3	20011115		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ,

PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1239890	A2	20020918	EP 2000-991148	200012 08
EP 1239890	B1	20041110		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003516813	T	20030520	JP 2001-544920	200012 08
AT 281847	T	20041115	AT 2000-991148	200012 08
ES 2231305	T3	20050516	ES 2000-991148	200012 08
US 20030068295	A1	20030410	US 2002-149564	200209 09
US 7157411	B2	20070102		
PRIORITY APPLN. INFO.:			US 1999-170424P P	199912 13
			WO 2000-EP12374 W	200012 08

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 135:66066

AB This invention relates to odor neutralizers comprising esters such as 2,4-dimethyl-3-pentyl esters of propionic, isobutyric, crotonic, and butyric acids. These esters and a number of other similar esters were prepared and tested for their deodorant properties against sweat, ammonia, tobacco smoke, etc.

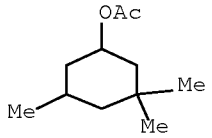
IT 67859-96-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(ester odor neutralizers)

RN 67859-96-5 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



IPCI A61L0009-01 [ICM,7]

IPCR A61K0008-00 [I,C*]; A61K0008-00 [I,A]; A61K0008-30 [I,C*];

A61K0008-30 [I,A]; A61K0008-37 [I,A]; A61L0009-01 [I,C*];
A61L0009-01 [I,A]; A61Q0005-00 [I,C*]; A61Q0005-00 [I,A];
A61Q0005-10 [I,C*]; A61Q0005-10 [I,A]; A61Q0007-00 [I,C*];
A61Q0007-00 [I,A]; A61Q0009-04 [I,C*]; A61Q0009-04 [I,A];
A61Q0015-00 [I,C*]; A61Q0015-00 [I,A]; C02F0001-00 [I,C*];
C02F0001-00 [I,A]; C11D0003-20 [I,C*]; C11D0003-20 [I,A]

CC 62-5 (Essential Oils and Cosmetics)
Section cross-reference(s): 23

IT 1637-22-5P 1637-24-7P 6070-14-0P 20777-45-1P 32376-43-5P
65466-77-5P 67859-96-5P 87386-67-2P 94021-79-1P
94200-12-1P 97766-62-6P 105937-88-0P 119617-64-0P
123232-56-4P 141553-01-7P 345288-58-6P 345288-59-7P
345288-60-0P 345288-61-1P 345288-62-2P 345288-63-3P
345288-64-4P 345288-65-5P 345288-66-6P 345288-67-7P
345288-68-8P 345288-69-9P 345288-70-2P 345288-71-3P
345288-72-4P 345288-73-5P 345288-74-6P 345288-75-7P
345288-76-8P 345288-77-9P 345288-78-0P 345288-79-1P
345288-80-4P 345288-81-5P 345288-82-6P 345288-83-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(ester odor neutralizers)

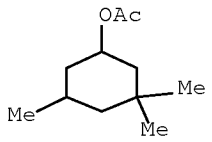
OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1986:33872 HCAPLUS Full-text
DOCUMENT NUMBER: 104:33872
ORIGINAL REFERENCE NO.: 104:5553a,5556a
TITLE: Ultraviolet absorbing compounds and compositions containing these compounds
INVENTOR(S): Baker, James Albert
PATENT ASSIGNEE(S): Graesser Laboratories Ltd., UK
SOURCE: Eur. Pat. Appl., 25 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 153089	A1	19850828	EP 1985-300800	19850206
R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
GB 2155467	A	19850925	GB 1985-3039	19850206
GB 2155467	B	19870325		
US 4592906	A	19860603	US 1985-699955	19850208
AU 8538675	A	19850822	AU 1985-38675	19850206

				13
ZA 8501081	A	19861029	ZA 1985-1081	
				198502
				13
JP 60231637	A	19851118	JP 1985-27539	
				198502
				14
PRIORITY APPLN. INFO.:			GB 1984-3836	A
				198402
				14

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 104:33872
AB 4-Me2NC6H4CH:CHCO2R (I; R = 2-ethylhexyl, 2-octyl) were prepared for use as UV (type A) absorbers in sunscreen compns. Thus, 40 g I (R = Et), 60 mL 2-ethylhexanol, 60 mL PhMe, and 0.1 g Na were stirred at 130° to give, after workup and vacuum distillation, 38 g I (R = 2-ethylhexyl; II). II has a m.p. of −5°, is completely miscible with both mineral oil and MeOH, and has an absorptivity of 101 at λmax = 363 nm. Several sun-block formulations were given.
IT 67859-96-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with dimethylaminobenzaldehyde)
RN 67859-96-5 HCAPLUS
CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



IPCI C07C0101-46 [ICM,4]; A61K0007-42 [ICS,4]
IPCR C09K0003-00 [I,C*]; C09K0003-00 [I,A]; A61K [I,S]; A61K0008-00 [I,C*]; A61K0008-00 [I,A]; A61K0008-30 [I,C*]; A61K0008-37 [I,A]; A61K0008-41 [I,A]; A61K0008-44 [I,A]; A61K0031-185 [I,C*]; A61K0031-195 [I,A]; A61Q0017-04 [I,C*]; A61Q0017-04 [I,A]; C07C0067-00 [I,C*]; C07C0067-00 [I,A]; C07C0227-00 [I,C*]; C07C0227-00 [I,A]; C07C0229-00 [I,C*]; C07C0229-44 [I,A]
CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 62
IT 112-06-1 112-14-1 112-17-4 123-92-2 2051-50-5 58430-94-7 67859-96-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with dimethylaminobenzaldehyde)
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

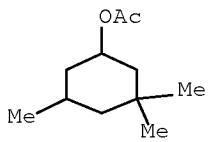
L4 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1959:94508 HCAPLUS Full-text
DOCUMENT NUMBER: 53:94508
ORIGINAL REFERENCE NO.: 53:17008i,17009a-d
TITLE: Stereochemistry of the dihydroisophorols
AUTHOR(S): Alkonyi, Istvan
CORPORATE SOURCE: Univ. Leipzig, Germany
SOURCE: Chemische Berichte (1959), 92, 1130-4

CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The dihydroisophorol (I), m. 34°, and the isomer (II), m. 56°, were identified chemically and spectroscopically as the cis and trans isomers, resp. The compound regarded by Knoevenagel [Ann. 297, 194(1897)] as I was identified as an acetylated product. I (7.6 g.) and 1.23 g. Na in 20 cc. C6H6 refluxed 2 hrs., treated with 7.6 g. phthalic anhydride (III) in 100 cc. C6H6, refluxed 5 hrs., poured into H2O acidified with HCl, and extracted with Et2O, the extract dried and evaporated, and the residue recrystd. from C6H6 and then EtOH gave 2.5 g. I acid phthalate (IV), m. 129°. II (10 g.) and 10 g. III in 30 cc. C6H6 refluxed 6.5 hrs., cooled, filtered from 1.6 g. unchanged III, and evaporated yielded 15.2 g. II acid phthalate (V), m. 120-1° (EtOH). I treated with Ac2O and KOAc gave the acetate (VI), b27 96-7°, n19D 1.4411, d19 0.9197. II yielded similarly the acetate (VII), b24 98-8.5°, n19D 1.4421, d19 0.9243. VI and VII (0.001 mole each) were treated with MeMgI according to the method of Treibs (C.A. 40, 53963) (millimoles MeMgI consumed after 3, 6, and 10 min. given): VI, 1.37, 1.47, 1.60; VII, 1.28, 1.32, 1.54. II (2 g.) and 1 g. Na heated 10 hrs. at 200° under N, treated with moist Et2O, and shaken with Et2O and dilute H2SO4, and the Et2O layer worked up yielded I, m. 34°. I (12 g.) in 18 cc. C5H5N treated slowly with cooling with 16.2 g. p-MeC6H4SO2Cl, kept 4 days at room temperature, poured into 113 g. 10% H2SO4, and filtered, and the crude product (11.6 g.) recrystd. from MeOH and then Me2CO yielded 5.9 g. I p-toluenesulfonate (VIII), m. 81°. The rates of hydrolysis were determined for the acid phthalates by treating 1.4516 g. ester with 0.05N H2SO4 (reaction time in hrs., and 2nd order rate consts. of IV and V given): 1, 4.5, 0.55; 1.5, 4.8, 0.56; 2, 5.0, 0.59; 2.5, 5.2, 0.60; 3, 5.5, 0.60; 3.5, 5.6, 0.62; 4.5, 6.1, 0.64; 5.5, 6.5, 0.67. The solvolysis of VIII in MeOH (and EtOH) at reflux temperature was measured by titrating aliquots of a solution of 0.5971 g. VIII in 100 cc. absolute MeOH at time intervals; the olefin content in the titrated, neutral reaction mixture was determined by further titration with 0.1N Br; the first-order rate consts., k + 102 after 1, 2, 3, and 4 hrs., resp., for the solvolysis in MeOH were 3.61, 3.62, 3.59, and 3.68 with a half-life of the ester of 19.2 hrs.; the values obtained for the ethanolysis were 5.11, 5.5, 5.87, and 5.85 + 10-2, resp., with a half-life of the VIII of 12.5 hrs.

IT 67859-96-5
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 67859-96-5 HCAPLUS
CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



CC 10D (Organic Chemistry: Alicyclic Compounds)
IT 67859-96-5 93157-19-8
(Derived from data in the 6th Collective Formula Index (1957-1961))

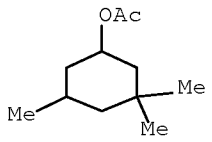
L4 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1959:94507 HCAPLUS Full-text
DOCUMENT NUMBER: 53:94507
ORIGINAL REFERENCE NO.: 53:17008c-i

TITLE: Elimination reaction. X. Pyrolysis of xanthate and sulfite esters of erythro- and threo-3-(p-tolylthio)- and 3-(p-tolylsulfonyl)-2-butanols
AUTHOR(S): Bordwell, F. G.; Landis, Phillip S.
CORPORATE SOURCE: Northwestern Univ., Evanston, IL
SOURCE: Journal of the American Chemical Society (1958), 80, 6383-6
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 53:94507

AB The study of elimination reactions has been extended to the acyclic systems. dl-threo-3-(p-Tolylthio)-2-butanol added to a stirred suspension of K in dry C6H6, the mixture stirred 2 hrs. at room temperature and 2 hrs. at 50-5°, CS2 added, the solution refluxed 8 hrs., MeI added, the solution stirred overnight, filtered, washed with H2O, dried, the solvent evaporated, the crude xanthate pyrolyzed 30 min. at 200°, and the products distilled gave dl-threo-3-(p-tolylthio)-2-butyl S-Me xanthate (XIII), b0.1 135-47°. XIII oxidized with 30% H2O2 in HOAc gave the sulfone, m. 35-45°, identified by its infrared spectrum as cis-2-(p-tolylsulfonyl)-2-butene (XIV); the strong 14.7 μ peak of the trans isomer was absent. The dl-erythro-isomer (XV) of XIII, similarly prepared and pyrolyzed, gave on oxidation mostly trans-2-(p-tolylsulfonyl)-2-butene (XVI), m. 45-7°. dl-threo-3-(p-Tolylsulfonyl)-2-butyl S-Me xanthate (XVII) similarly prepared and pyrolyzed gave 58% XIV, b0.5 145-55°, and no more than 5% trans isomer. The dl-erythro isomer (XVIII) of XVII gave on pyrolysis an oil, b2 145-75°; on fractionation by chromatographing over silica gel, a mixture of 80% XIV and 20% XVI was identified by infrared analysis. Pyrolysis of 6.5 g. XVII and 2.0 g. XVI, gave 5.3 g. mixture containing approx. 40% XVI vs. the calculated 30%, if no rearrangement had occurred. threo- and erythro-3-(p-Tolylsulfonyl)-2-butanol were treated with K in C6H6, the suspension shaken with 10% HCl, the C6H6 layer separated, washed with H2O, dried, and the C6H6 evaporated The infrared spectrum from the erythro isomer showed no threo present (absence of 2 strong doublets at 10.18, 10.38 and 10.85, 11.05 μ); the strong band at 9.98 μ characteristic of the erythro-alc. was absent in the recovered threo-alc. XVI refluxed 30 min. with tert-BuOH containing K, the cooled solution poured into H2O, and extracted with CHCl3 gave on evaporation of CHCl3 a mixture identified by infrared analysis as 80% XIV and 20% XVI; further treatment with K-containing tert-BuOH gave pure XIV. XIV was unchanged on similar treatment. Me erythro-3-(p-tolylthio)-2-butyl sulfite (XIX) pyrolyzed in vacuo at 200-20° gave 97% distillate; the latter, oxidized with H2O2 gave a solid, m. 35-43°, identified by infrared analysis as a mixture of 25% XVI and 75% XIV. The strong 14.7 μ band of the trans isomer did not occur in the pyrolysis product from the threo isomer of XIX. Me erythro-3-(p-tolylsulfonyl)-2-butyl sulfite (XX) heated 30 min. at 170° under N and the product distilled in vacuo gave a product, b0.4 160-4°; after chromatographing over silica gel a mixture of 15% XVI and 85% XIV was obtained. Pyrolysis of the threo isomer of XX gave 10% XVI and 90% XIV. Since stereoselective cis elimination occurred in the pyrolysis of XIII and XV, with the formation of XIV and XVI, while XVII and XVIII gave on pyrolysis only the more stable isomer, XIV, it is concluded that the mechanism is a stepwise one, involving a polar intermediate which can undergo rotation prior to forming olefin. XX and its threo isomer both gave XIV on pyrolysis, indicating a similar mechanism. An acid-catalyzed rearrangement of one of the olefins is believed responsible for the identity of pyrolysis products from XIX and its threo isomer.

IT 67859-96-5
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 67859-96-5 HCAPLUS
CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



CC 10D (Organic Chemistry: Alicyclic Compounds)
IT 67859-96-5 93157-19-8
(Derived from data in the 6th Collective Formula Index (1957-1961))

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